

# Phase-Space Functions and Energy Densities

Michael Springborg

Physical Chemistry,  
University of Saarland,  
66123 Saarbrücken, Germany

[m.springborg@mx.uni-saarland.de](mailto:m.springborg@mx.uni-saarland.de)

<http://www.uni-saarland.de/fak8/springborg.html>

Most often quantum mechanics is formulated in position space. Then, observables are in the general case expressed through operators. Alternatively, by formulating quantum mechanics in phase space observables are functions and expectation values are expressed in terms of integrals over phase space. This permits definitions of position-space densities for any state and property. However, the fact that the correspondence between classical functions and quantum-mechanical operators is non-unique leads to non-unique definitions of phase-space and, consequently, position-space densities.

In this contribution we shall argue that the Weyl correspondence and the accompanying Wigner phase-space function possess particularly appealing properties. Subsequently, we shall give explicit results for energy densities in the position space obtained with this correspondence rule and compare it with those obtained with other correspondence rules. Special emphasis is put on kinetic- and exchange-energy densities. It is shown that the Weyl correspondence leads to a maximally localized exchange hole. Numerical results for energy densities for 15 closed-shell atoms are presented and it is analyzed whether the results can be approximated through more or less local functions of the electron density and/or the Kohn-Sham orbitals.

Further reading:

M. Springborg and J. P. Dahl, J. Chem. Phys. **110**, 9360 (1999)

M. Springborg, Chem. Phys. Lett. **308**, 83 (1999)

M. Springborg, J. P. Perdew, and K. Schmidt, Z. Phys. Chem. **215**, 1243 (2001)